

IN THE CLAIMS

Please cancel claims 1-22 and 26.

Please amend claim 23 as follows:

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23. (Amended) A method for evaluating the ability of a chemical entity to associate with a molecule or molecular complex comprising all or any part of a binding pocket defined by structure coordinates of IMPDH amino acids 68, 69, 93, 273, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 330, 331, 332, 333, 334, 337, 339, 340, 364, 413, 414, 415, 416, 420, 439, 440, 441, 442, 469, and 470 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

- a. employing computational means to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex; and
- b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket.

Please add claims 27-36 as follows:

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27. (Added) The method according to claim 23, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 274, 275, 276, 277, 303, 322, 324, 325, 326, 331, 333, 414, 415, and 441 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket

that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

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28. (Added) The method according to claim 27, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 275, 276, 303, 325, 326, 331, 333 and 441 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

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29. (Added) A method for evaluating the ability of a chemical entity to associate with a molecule or molecular complex comprising all or any parts of a binding pocket defined by structure coordinates of IMPDH amino acids 67, 68, 69, 70, 73, 274, 275, 276, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 440, 441, 442, 443, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

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- a. employing computational means to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex; and
 - b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket.

30. (Added) The method according to claim 29, wherein said binding

pocket is defined by structure coordinates of IMPDH amino acids 68, 69, 70, 303, 322, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 419, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

31. (Added) The method according to claim 30, wherein said binding

pocket is defined by structure coordinates of IMPDH amino acids 68, 70, 322, 328, 329, 331, 332, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

32. (Added) The method according to claim 29, wherein said binding

pocket is defined by structure coordinates of IMPDH amino acids 67, 68, 69, 70, 73, 93, 273, 274, 275, 276, 277, 303, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 337, 339, 340, 364, 365, 366, 367, 368, 385, 386, 387, 388, 389, 391, 411, 412, 413, 414, 415, 416, 419, 420, 439, 440, 441, 442, 443, 469, 470, 500, 501, 502, 503, 504, 505, and 506 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

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33. (Added) The method according to claim 32, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 68, 69, 70, 274, 275, 276, 277, 303, 322, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 335, 364, 365, 366, 367, 385, 386, 387, 388, 411, 413, 414, 415, 416, 441, 442, 443, 501, 502, 503, and 504 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

34. (Added) The method according to claim 33, wherein said binding pocket is defined by structure coordinates of IMPDH amino acids 68, 70, 275, 276, 303, 322, 325, 326, 328, 329, 331, 332, 333, 335, 364, 366, 387, 388, 411, 413, 414, 415, 441, 442, 501, and 502 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

35. (Added) The method according to claim 32, wherein said molecule or molecular complex is defined by the set of structure coordinates according to Figure 1, or a homologue thereof, wherein said homologue has a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5 Å.

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36. (Added) The method according to claim 32, wherein said molecule or molecular complex comprises amino acids 1-514 of IMPDH, XMP*, and MPA.